Cyclopentane

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 2.78

Global applicability domain: Inside

Local applicability domain index: 9.90e-01

Confidence level: 8.19e-01

Nearest Neighbors from the Training Set

Image not found
Isopropyl acetate
Measured: 2.93
Predicted: 2.76

Image not found
1-Chlorobutane
Measured: 2.72
Predicted: 2.78

Image not found
1-Hexene
Measured: 2.41
Predicted: 2.75

Image not found
3-Methyl-2-butanone
Measured: 3.04
Predicted: 2.75

Image not found
Carbon tetrachloride
Measured: 2.79
Predicted: 2.78